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# Commutators with maximal Frobenius norm

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ABSTRACT

It is known that for any nonzero complex $n \times n$ matrices $X$ and $Y$ the quotient of Frobenius norms

$$\frac{\|XY - YX\|_F}{\|X\|_F\|Y\|_F}$$

does not exceed $\sqrt{2}$. However, except for some special cases, only necessary conditions for attaining this bound have been found so far. We will completely characterize the pairs of matrices that satisfy equality with the quotient's maximum.



## 1. Introduction

We are looking at the inequality

$$\|XY - YX\|_F^2 \leqslant 2\|X\|_F^2\|Y\|_F^2, \tag{1}$$

which was conjectured by Böttcher and one of the authors [3] to be valid for real square matrices $X$ and $Y$ and the Frobenius norm $\|\cdot\|_F$. The conjecture was shown to be true for $3 \times 3$ matrices by László [6], and in general by Jin and one of the authors [8] and Lu [7]. The validity has been extended even to complex matrices by Böttcher and one of the authors [4]. Recently, another proof of this result by Audenaert [2] appeared.

Although there are now four completely different proofs, the equality cases of (1) do not follow readily. In [4], Böttcher and one of the authors gave necessary conditions and obtained characterizations for some particular classes of matrices $X$ and $Y$. In accordance with the notation of that paper we call a pair $(X, Y)$ of nonzero matrices maximal if it satisfies (1) with an equality sign. We will determine all maximal pairs of complex, as well as real matrices without any additional constraints.

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Throughout this paper we will work over the field $\mathbf{C}$ of complex numbers. Nevertheless, we will embark on necessary modifications for the real case. By $M_{m,n}$ we denote the vector space of all $m \times n$ matrices with complex entries. We also write $M_n = M_{n,n}$ for the space of square matrices and $\mathbf{C}^n = M_{n,1}$ for the space of columns. The identity matrix of order $n$ is denoted by $I_n$, and $O$ will indicate zero matrices of appropriate order (depending on the context). For $X \in M_{m,n}$, the conjugate, transpose and adjoint of $X$ are referred to as $\overline{X}, X^t$ and $X^*$, respectively.

The vector space $M_{m,n}$ is equipped with the usual inner product $\langle X, Y\rangle = \operatorname{tr}(Y^*X)$, where $\operatorname{tr} X$ denotes the trace of $X$. Then, the Frobenius norm of $X$ is given by $\|X\|_{\mathsf{F}} = \sqrt{\langle X, X\rangle}$. Whenever $X$ and $Y$ are orthogonal, i.e. $\langle X, Y\rangle = 0$, we write $X \perp Y$. The Lie bracket serves as an abbreviation for the commutator $[X, Y] = XY - YX$ of two square matrices and we will also use the direct sum notation

$$A \oplus B = \begin{pmatrix} A & O \\ O & B \end{pmatrix}.$$

## 2. Some useful results on maximality

Let us first repeat some known properties of maximal pairs.

**Proposition 2.1** [4, Proposition 4.4, Corollary 4.2]. *Let $n > 1$ and $X, Y \in M_n$ be nonzero. Then the following assertions hold*:

(a) *For $n = 2$, $(X, Y)$ is a maximal pair if and only if* $\operatorname{tr} X = \operatorname{tr} Y = 0$ *and* $X \perp Y$.
(b) *If $(X, Y)$ is a maximal pair, then*

(i) $\operatorname{rank} X \leqslant 2$ *and* $\operatorname{rank} Y \leqslant 2$,
(ii) $\operatorname{tr} X = \operatorname{tr} Y = 0$,
(iii) $X \perp Y$,
(iv) $X \perp Y^m$ *and* $X^m \perp Y$ $(m = 2, 3, \ldots)$.

The following two statements give insight into the behaviour of maximality and will be advantageous later on. For this, we rely on block matrix structures

$$X = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

with a square matrix $A$ and utilize the knowledge of several blocks.

**Lemma 2.2.** *Let $n \geqslant 3$ and $X, Y \in M_n \setminus \{O\}$.*

(a) *Suppose that*

$$X = \begin{pmatrix} A & O \\ O & O \end{pmatrix} \quad \text{and} \quad Y = \begin{pmatrix} E & F \\ G & H \end{pmatrix}$$

*with $A, E \in M_r$ for some $1 \leqslant r < n$. Then $(X, Y)$ is a maximal pair if and only if $F, G$ and $H$ are all zero matrices and $(A, E)$ is maximal.*
(b) *Suppose that*

$$X = \begin{pmatrix} A & O \\ C & O \end{pmatrix} \quad \text{and} \quad Y = \begin{pmatrix} E & O \\ G & O \end{pmatrix}$$

*with $A, E \in M_r$ for some $1 \leqslant r < n$. Then $(X, Y)$ is a maximal pair if and only if $C = G = O$ and $(A, E)$ is maximal.*

**Proof.** Take a look at (a). A direct computation shows

$$\|XY - YX\|_{\mathsf{F}}^2 = \|AE - EA\|_{\mathsf{F}}^2 + \|AF\|_{\mathsf{F}}^2 + \|GA\|_{\mathsf{F}}^2 \tag{2}$$

$$\leqslant 2\|A\|_F^2\|E\|_F^2 + \|A\|_F^2\|F\|_F^2 + \|G\|_F^2\|A\|_F^2$$

by using the commutator bound (1) and the submultiplicativity of the Frobenius norm (see e.g. [5, p. 291]). On the other hand we have

$$2\|X\|_F^2\|Y\|_F^2 = 2\|A\|_F^2\left(\|E\|_F^2 + \|F\|_F^2 + \|G\|_F^2 + \|H\|_F^2\right). \tag{3}$$

The maximality of $(X, Y)$, i.e. equality of (2) and (3), then yields

$$\|A\|_F^2\left(\|F\|_F^2 + \|G\|_F^2 + 2\|H\|_F^2\right) \leqslant 0$$

and therefore, $F, G$ and $H$ necessarily are zero matrices. As a consequence, (2) and (3) simplify to $\|XY - YX\|_F^2 = \|AE - EA\|_F^2$ and $2\|X\|_F^2\|Y\|_F^2 = 2\|A\|_F^2\|E\|_F^2$, respectively. Hence, we obtain the maximality of $(A, E)$. Clearly, the converse implication is true.

Now, for the proof of (b), another calculation (involving moreover the triangle inequality) yields

$$\begin{aligned}\|XY - YX\|_F^2 &= \|AE - EA\|_F^2 + \|CE - GA\|_F^2\\ &\leqslant 2\|A\|_F^2\|E\|_F^2 + (\|CE\|_F + \|GA\|_F)^2\\ &\leqslant 2\|A\|_F^2\|E\|_F^2 + (\|C\|_F\|E\|_F + \|G\|_F\|A\|_F)^2.\end{aligned}$$

On the other hand we get

$$2\|X\|_F^2\|Y\|_F^2 = 2\left(\|A\|_F^2 + \|C\|_F^2\right)\left(\|E\|_F^2 + \|G\|_F^2\right).$$

Similarly to the proof of (a), we obtain

$$2\|A\|_F^2\|E\|_F^2 + (\|C\|_F\|E\|_F + \|G\|_F\|A\|_F)^2 \geqslant 2\left(\|A\|_F^2 + \|C\|_F^2\right)\left(\|E\|_F^2 + \|G\|_F^2\right),$$

which gives

$$0 \geqslant (\|C\|_F\|E\|_F - \|G\|_F\|A\|_F)^2 + 2\|C\|_F^2\|G\|_F^2.$$

Thus, we can easily deduce that $C = G = O$. The remainder is as for the previous statement. □

We remark that the proof indeed handles the case $r = 1$, too. However, a pair $(A, E)$ of scalars will never be maximal.

If $x, y \in \mathbf{C}^n$ are orthogonal vectors of the same length, then $x + y$ and $x - y$ are also orthogonal. This property carries over to the linear combinations $\alpha x + \beta y$ and $\bar\beta x - \bar\alpha y$ with $\alpha, \beta \in \mathbf{C}$, as well. The subsequent proposition works in a similar fashion.

**Proposition 2.3.** *Let $n > 1$ and $X, Y \in M_n \setminus \{O\}$. Suppose that $\|X\|_F = \|Y\|_F$ and $(X, Y)$ is a maximal pair. Then for any $\alpha, \beta \in \mathbf{C}$ not both zero, the pair $(\alpha X + \beta Y, \bar\beta X - \bar\alpha Y)$ is also maximal.*

**Proof.** Property (iii) of Proposition 2.1(b) ensures $X \perp Y$ for any maximal pair. This orthogonality and the equality of norms yield

$$\begin{aligned}&\frac{\|(\alpha X + \beta Y)(\bar\beta X - \bar\alpha Y) - (\bar\beta X - \bar\alpha Y)(\alpha X + \beta Y)\|_F^2}{\|\alpha X + \beta Y\|_F^2\|\bar\beta X - \bar\alpha Y\|_F^2}\\ &= \frac{\left(|\alpha|^2 + |\beta|^2\right)^2\|XY - YX\|_F^2}{\left(|\alpha|^2\|X\|_F^2 + |\beta|^2\|Y\|_F^2\right)\left(|\beta|^2\|X\|_F^2 + |\alpha|^2\|Y\|_F^2\right)}\\ &= \frac{\|XY - YX\|_F^2}{\|X\|_F^2\|Y\|_F^2}.\end{aligned}$$

Hence, the two pairs are maximal simultaneously. □

Note that under the assumptions of Proposition 2.3, the orthogonality of $\alpha X + \beta Y$ and $\bar{\beta}X - \bar{\alpha}Y$ with $\alpha = 1$ and $\beta = 0$ automatically implies the orthogonality of $X$ and $Y$. So, the result is actually an equivalence.

The idea of the following proposition is inspired by the work of Lu [7]. Though only real matrices are considered there, the statement is more general and can be extended to complex matrices. For this, replace the $T$ in Lemma 3 of [7] by the mapping $Y \mapsto [X^*, [X, Y]]$. Later we will base a fundamental statement upon that result.

**Proposition 2.4.** *Let $n > 1$ and $X, Y \in M_n$ with $\|X\|_{\mathsf{F}} = \|Y\|_{\mathsf{F}} = 1$. Set $Z = \frac{1}{\sqrt{2}}[X^*, Y^*]$. If $(X, Y)$ is maximal, then*

(i) $\|Z\|_{\mathsf{F}} = 1$,
(ii) *$Z \perp X$ and $Z \perp Y$,*
(iii) *the pairs $(X, Z)$ and $(Y, Z)$ are maximal.*

*Moreover, we have*

(iv) *$[X, Y] \perp [X, Z]$ and $[X, Y] \perp [Y, Z]$.*

*Consequently,*

(v) *the pair $(X, \beta Y + \gamma Z)$ is maximal for any $\beta, \gamma \in \mathbf{C}$ with $|\beta|^2 + |\gamma|^2 > 0$.*

**Proof.** Although some of the statements are taken from [7], we will verify the claims directly. The maximality of $(X, Y)$ is synonymous to the maximality of $(X^*, Y^*)$ and ensures $\|[X^*, Y^*]\|_{\mathsf{F}}^2 = 2$, which implies (i).

With regard to (ii), first observe $Z^* = -[X, Y]/\sqrt{2}$. Then, a straight-forward inspection yields the orthogonality $Z \perp X$:

$$\begin{aligned}\langle X, -\sqrt{2}Z\rangle &= \operatorname{tr}\left(-\sqrt{2}Z^*X\right) = \operatorname{tr}\ ((XY - YX)X) \\ &= \operatorname{tr}\ (X(YX)) - \operatorname{tr}\ (YXX) = \operatorname{tr}\ ((YX)X) - \operatorname{tr}\ (YXX) = 0\end{aligned}$$

due to the additivity of the trace and the identity $\operatorname{tr}(AB) = \operatorname{tr}(BA)$ (see e.g. [5, p. 42]).

For (iii), the maximality of $(X, Y)$ implies

$$2 = \|[X, Y]\|_{\mathsf{F}}^2 = \langle XY - YX, -\sqrt{2}Z^*\rangle$$

and consequently,

$$\begin{aligned}\sqrt{2} &= \langle YX, Z^*\rangle - \langle XY, Z^*\rangle = \langle Y, Z^*X^*\rangle - \langle Y, X^*Z^*\rangle \\ &\leqslant \|Y\|_{\mathsf{F}}\|Z^*X^* - X^*Z^*\|_{\mathsf{F}}\end{aligned}$$

by properties of the inner product and Cauchy's inequality. By our assumptions, (i) and (1), we then have

$$\sqrt{2} \leqslant \|XZ - ZX\|_{\mathsf{F}} \leqslant \sqrt{2},$$

which is the maximality of $(X, Z)$.

The claims (ii) and (iii) for $(Y, Z)$ follow by swapping the roles of $X$ and $Y$. Substituting $[X, Y]$ with $-\sqrt{2}Z^*$, the proof of (iv) is as for (ii).

Finally, (v) is a consequence of properties (i) to (iv) and the Pythagorean theorem for the Frobenius norm:

$$\frac{\|[X,\beta Y+\gamma Z]\|_F^2}{\|X\|_F^2\|\beta Y+\gamma Z\|_F^2}=\frac{\|[X,\beta Y]\|_F^2+\|[X,\gamma Z]\|_F^2}{|\beta|^2+|\gamma|^2}=2. \qquad \square$$

Note that by (iii) and Proposition 2.1(b)(iii), condition (ii) is valid without the necessity of a separate proof. We remark that the proof of (iii), more precisely the requirement of equality in Cauchy's inequality, unveils the linear dependency of $Y$ and $[X^*, Z^*]$ for any maximal pair. This relation was obtained in [7] by means of eigenvalues and was also encountered in Section 2 of [9].

The next result is technical but of service in connection with the previous two propositions.

**Lemma 2.5.** *Let $n \geqslant 3$ and $X, Y \in M_n$. Suppose $X = (x_1, x_2, 0, \ldots, 0)$ and $Y = (y_1, y_2, \ldots, y_n)$ with columns $x_i, y_i \in \mathbf{C}^n$. If $\operatorname{rank}(\alpha X + \beta Y) = 2$ for all $\alpha, \beta \in \mathbf{C}$ not both zero, then $y_3, \ldots, y_n \in \operatorname{span}\{x_1, x_2\}$.*

**Proof.** Let $V \in M_n$ be a unitary matrix such that its first two columns $v_1$ and $v_2$ satisfy

$$\operatorname{span}\{v_1, v_2\} = \operatorname{span}\{x_1, x_2\}.$$

Keep in mind that $\operatorname{rank} X = 2$ is given. Then write

$$V^*X = \widehat{X}_0 \oplus O \quad \text{and} \quad V^*Y = (\hat{y}_{ij})_{i,j=1}^n,$$

with $\widehat{X}_0 \in M_2$. It now suffices to show $\hat{y}_{ij} = 0$ for all $i, j = 3, \ldots, n$.

Fix any $3 \leqslant i, j \leqslant n$ and let $\alpha \in \mathbf{C}$ be arbitrary. Without restriction we assume $\beta = 1$. By $S_{i,j}(\alpha)$ we denote the $3 \times 3$ matrix formed by the intersection of the first, second and $i$th rows and first, second and $j$th columns of $\alpha V^*X + V^*Y$. Using the assumption that any nonzero linear combination of $X$ and $Y$ is of rank two, we have

$$\det \widehat{X}_0 \neq 0 \quad \text{and} \quad 0 = \det S_{i,j}(\alpha) = \hat{y}_{ij}(\det \widehat{X}_0)\alpha^2 + a\alpha + b, \tag{4}$$

where $a$ and $b$ are constants depending, of course, on $i$ and $j$, but that are independent of $\alpha$. As (4) holds for all $\alpha \in \mathbf{C}$, we have $\hat{y}_{ij} = 0$ and the claim follows. $\square$

Before proceeding with the characterization of maximality, we will take a closer look at the already treated special cases.

**Example 2.6.** From Proposition 4.6 of [4] we know a characterization of maximal pairs consisting of at least one normal matrix. It is proven that if $X \in M_n$ is normal, the pair $(X, Y)$ is maximal if and only if there exists a unitary matrix $U \in M_n$ such that

$$X = U(X_0 \oplus O)U^* \quad \text{and} \quad Y = U(Y_0 \oplus O)U^*, \tag{5}$$

where

$$X_0 = \begin{pmatrix} \lambda & 0 \\ 0 & -\lambda \end{pmatrix} \quad \text{and} \quad Y_0 = \begin{pmatrix} 0 & a \\ b & 0 \end{pmatrix},$$

with some complex numbers $\lambda \neq 0$ and $a, b$ $(|a|^2 + |b|^2 > 0)$.

Gathering the facts that matrices of a maximal pair have trace zero, are orthogonal (see properties (ii) and (iii) of Proposition 2.1(b)) and are determined by these properties in the case of $2 \times 2$ matrices (Proposition 2.1(a)), together with the well-known unitary diagonizability of normal matrices (see e.g. [5, p. 101]), one can deduce the following.

*Suppose $X \in M_n$ is normal.*
*A pair $(X, Y)$ is maximal if and only if there is a unitary $U$ such that (5) holds with a maximal pair $(X_0, Y_0)$ of $2 \times 2$ matrices.*
*Here, $X_0$ is normal, too.*

In view of property (i) in Proposition 2.1(b) we guess that such a result can be shown for any pair of matrices (without the assumption that $X$ is normal). As the Frobenius norm is unitarily invariant, i.e.

$$\|UA\|_F = \|AV\|_F = \|A\|_F \quad \text{for any } U, V \text{ unitary and } A \in M_{m,n},$$

the pair $(U^*XU, U^*YU)$ is maximal whenever $(X, Y)$ is maximal. So, the claim is trivial for $n = 2$.

We want to study another class of matrices.

**Example 2.7.** In [4], Proposition 4.5 characterizes all maximal pairs $(X, Y)$ of two rank one matrices by

$$\operatorname{tr} X = 0 \quad \text{and} \quad Y = \alpha X^* \quad \text{for some } \alpha \neq 0.$$

Our guess is correct in that case. To this end, write $X = ab^*$ with $a, b \in \mathbf{C}^n$ and $a^*b = \overline{\operatorname{tr} X} = 0$. Then we are able to create the claimed structure since

$$X = \begin{pmatrix} \frac{a}{\|a\|} & \frac{b}{\|b\|} \end{pmatrix} \begin{pmatrix} 0 & \|a\|\|b\| \\ 0 & 0 \end{pmatrix} \begin{pmatrix} a^*/\|a\| \\ b^*/\|b\| \end{pmatrix},$$

$\frac{a}{\|a\|}$ and $\frac{b}{\|b\|}$ are othonormal and can thus be extended by $n - 2$ columns to form a unitary matrix. For the converse, it suffices to convince oneself that any $2 \times 2$ matrix with trace zero and rank one is unitary similar to a matrix

$$\begin{pmatrix} 0 & x \\ 0 & 0 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 0 & 0 \\ y & 0 \end{pmatrix}.$$

Putting all these pieces together we obtain the following.

*Suppose* $\operatorname{rank} X = \operatorname{rank} Y = 1$.
*A pair* $(X, Y)$ *is maximal if and only if there is a unitary* $U$ *such that* (5) *holds with a maximal pair* $(X_0, Y_0)$ *of* $2 \times 2$ *matrices.*
*Here, we also have* $\operatorname{rank} X_0 = \operatorname{rank} Y_0 = 1$.

Naturally, these two examples are heavily indicating the general validity of our guess. Moreover, the claim is compatible with the known necessary conditions.

Observe that (5) forces rank at most two for both matrices $X$ and $Y$, yielding property (i) of Proposition 2.1(b). Unitary similarity preserves the trace [5, p. 46], so property (ii) is also transferred from $X_0$ and $Y_0$ to $X$ and $Y$. For property (iii), write

$$\operatorname{tr}(Y^*X) = \operatorname{tr}\left(U(Y_0^* \oplus O)(X_0 \oplus O)U^*\right) = \operatorname{tr}(Y_0^*X_0 \oplus O) = \operatorname{tr}(Y_0^*X_0)$$

and link the orthogonality of both pairs. Similarly, for the preservation of property (iv) one may use the fact

$$X^2 = U(X_0^2 \oplus O)U^*.$$

**Remarks**. A characterization by means of (5) is especially beautiful, since Proposition 2.1(a) then will fix all maximal pairs $(X_0, Y_0)$ of $2 \times 2$ matrices.

All the results of this section can be read in the same way if the underlying field is given by the real numbers $\mathbf{R}$. In that case taking the conjugate has no effect and the adjoint in Proposition 2.4 may be replaced by the transpose.

Of course, the words "unitary matrix" in the proof of Lemma 2.5 and the two examples must be substituted by "orthogonal matrix". The necessary facts we referred to stay valid in that case.

## 3. The characterization of maximal pairs and its proof

This section is devoted to the proof of the general result.

**Theorem 3.1.** *Let* $n > 1$ *and* $X, Y \in M_n \setminus \{O\}$. *Then* $(X, Y)$ *is maximal if and only if there exists a unitary* $U \in M_n$ *such that*

$$X = U(X_0 \oplus O)U^* \quad \textit{and} \quad Y = U(Y_0 \oplus O)U^*$$

*with a maximal pair* $(X_0, Y_0)$ *of matrices*

$$X_0, Y_0 \in M_2. \tag{6}$$

With help of Proposition 2.1(a) the theorem above can immediately be rewritten as follows.

**Theorem 3.2.** *Let* $n > 1$ *and* $X, Y \in M_n \setminus \{O\}$. *Then* $(X, Y)$ *is maximal if and only if*

(i) *X and Y are simultaneously unitarily similar to matrices in* $M_2 \oplus O$,
(ii) $\operatorname{tr} X = \operatorname{tr} Y = 0$ *and*
(iii) $X \perp Y$.

We will prove Theorem 3.1 in several steps by the following propositions. Taking into account the unitary invariance of the Frobenius norm, it is clear that the "if" part is true and only the "only if" part requires an investigation. We will concentrate upon this implication exclusively in the subsequent proofs.

First of all, we give a generalization of the result mentioned in Example 2.7 and get rid of the requirement that both matrices are of rank one.

**Proposition 3.3.** *Theorem* 3.1 *is true if* $\operatorname{rank} X = 1$.

**Proof.** Suppose $(X, Y)$ is maximal and $\operatorname{rank} X = 1$. As already demonstrated in Example 2.7, there exists a unitary $U \in M_n$ such that

$$U^*XU = X_0 \oplus O \quad \text{with } X_0 \in M_2.$$

Due to the unitary invariance of the Frobenius norm, the pair $(U^*XU, U^*YU)$ is again maximal. From Lemma 2.2(a) we infer $U^*YU = Y_0 \oplus O$ for some $Y_0 \in M_2$, where $(X_0, Y_0)$ is maximal, too. □

**Remark.** As $\operatorname{rank} X = \operatorname{rank} X_0 = 1$, upon a unitary similarity of the form $V \oplus I_{n-2}$, we may further assume (for some numbers $x, y, z \in \mathbf{C}$)

$$X_0 = \begin{pmatrix} 0 & x \\ 0 & 0 \end{pmatrix}. \quad \text{As a consequence, } Y_0 = \begin{pmatrix} y & 0 \\ z & -y \end{pmatrix}$$

is given by the restrictions of Proposition 2.1(a).

Next, we will present a more sophisticated extension of Proposition 3.3 that is essentially based on Proposition 2.4. It will play a fundamental role for the remaining steps in the proof of the main result.

**Corollary 3.4.** *Let Z be given as in Proposition* 2.4. *Theorem* 3.1 *is true if*

$$\operatorname{rank}(\alpha X + \beta Y + \gamma Z) = 1$$

*for some complex numbers* $\alpha, \beta, \gamma$ *not all zero.*

**Proof.** Assume without loss of generality that $\|X\|_\mathsf{F} = \|Y\|_\mathsf{F} = 1$. Let $\alpha = 0$. If $\operatorname{rank}(\beta Y + \gamma Z) = 1$ for some $\beta, \gamma \in \mathbf{C}$, then by Proposition 2.4, $(X, \beta Y + \gamma Z)$ is maximal and thus Proposition 3.3 grants the existence of a unitary $U$ with

$$U^*XU = X_0 \oplus O \quad \text{and} \quad U^*(\beta Y + \gamma Z)U = W_0 \oplus O \quad (X_0, W_0 \in M_2).$$

As the pair $(U^*XU, U^*YU)$ is also maximal, Lemma 2.2(a) gives $U^*YU = Y_0 \oplus O$ with $Y_0 \in M_2$.

More generally, suppose $\operatorname{rank}(\alpha X + \beta Y + \gamma Z) = 1$ for some $\alpha, \beta, \gamma \in \mathbf{C}$ with $\alpha \neq 0$ and $\beta, \gamma$ not both zero (the case $\beta = \gamma = 0$ is already covered by Proposition 3.3). Put

$$\delta = \sqrt{|\beta|^2 + |\gamma|^2} \quad \text{and} \quad W = \frac{1}{\delta}(\beta Y + \gamma Z).$$

Then we have $\operatorname{rank}(\alpha X + \delta W) = 1$ and $\|X\|_\mathsf{F} = \|W\|_\mathsf{F} = 1$. By Proposition 2.4, $(X, W)$ is maximal and by Proposition 2.3, likewise $(\alpha X + \delta W, \delta X - \bar{\alpha} W)$. Now, by Proposition 3.3, there is a unitary $U$ such that

$$U^*(\alpha X + \delta W)U \quad \text{and} \quad U^*(\delta X - \bar{\alpha} W)U$$

are of the form $A \oplus O$ with $A \in M_2$. Consequently, $U^*XU$ and $U^*YU$ are also of such form. For the latter, consider e.g.

$$\left(\frac{\alpha}{\delta} + \frac{\delta}{\bar{\alpha}}\right) U^*XU = U^*\left(\frac{\alpha X + \delta W}{\delta} + \frac{\delta X - \bar{\alpha} W}{\bar{\alpha}}\right)U,$$

where $\frac{\alpha}{\delta} + \frac{\delta}{\bar{\alpha}} = \frac{|\alpha|^2 + \delta}{\delta \bar{\alpha}} \neq 0.$ $\square$

**Remark.** Be aware that Propositions 2.3 and 2.4, together with property (i) of Proposition 2.1(b) imply

$$\text{rank}\,(\alpha X + \beta Y + \gamma Z) \leqslant 2$$

for any maximal pair $(X, Y)$. This follows since $\alpha X + \beta Y + \gamma Z$ is part of a maximal pair, as demonstrated in the proof of Corollary 3.4.

The following step takes us quite the whole way with merely little effort. For this treatment, we need the notion of the kernel of a matrix $A \in M_n$, i.e. the set $\ker A = \{x \in \mathbf{C}^n : Ax = 0\}$.

**Proposition 3.5.** *When $n \geqslant 4$, Theorem 3.1 is true if (6) is replaced by $X_0, Y_0 \in M_4$.*

**Proof.** There is nothing to prove for $n = 4$. Hence, suppose $n > 4$. If $(X, Y)$ is maximal, the first property of Proposition 2.1(b) causes at most two-dimensional images for $X$ and $Y$, yielding

$$\dim(\ker X \cap \ker Y) \geqslant n - 4.$$

So, with a suitable unitary similarity on $X$ and $Y$, we may assume

$$U^*XU = \begin{pmatrix} X_0 & O \\ X_1 & O \end{pmatrix} \quad \text{and} \quad U^*YU = \begin{pmatrix} Y_0 & O \\ Y_1 & O \end{pmatrix}$$

with $X_0, Y_0 \in M_4$ and $X_1, Y_1 \in M_{n-4,4}$. Then by Lemma 2.2(b), we obtain $X_1 = Y_1 = O$ and the maximality of $(X_0, Y_0)$. $\square$

We remark that the proof of Proposition 3.5 is not reliant on Proposition 3.3 and the statements are not correlated.

Because of the last result, it suffices to prove Theorem 3.1 for $n \leqslant 4$. With the following result we gain one more order. This is where Corollary 3.4 comes into play. In what follows we suppose without restriction

$$\text{rank}\,X = \text{rank}\,Y = 2.$$

**Proposition 3.6.** *When $n = 4$, Theorem 3.1 is true with $X_0, Y_0 \in M_3$ instead of (6).*

**Proof.** Suppose $n = 4$. As $\text{rank}\,X = 2$, upon unitary similarity on $X$ and $Y$, we may assume

$$X = (x_1, x_2, 0, 0) \quad \text{and} \quad Y = (y_1, y_2, y_3, y_4)$$

with columns $x_i, y_i \in \mathbf{C}^4$. If $\text{rank}\,(\alpha X + \beta Y) = 1$ for some $\alpha, \beta \in \mathbf{C}$, Corollary 3.4 directly leads to the desired assertion. Thus, as remarked thereafter, we assume $\text{rank}\,(\alpha X + \beta Y) = 2$ for any $\alpha, \beta \in \mathbf{C}$ not both zero. From Lemma 2.5 we infer

$$y_3, y_4 \in \text{span}\{x_1, x_2\}.$$

Firstly, suppose $y_3$ and $y_4$ are linearly independent. As $\text{rank}\,Y = 2$, we even have $y_1, y_2 \in \text{span}\{x_1, x_2\}$. Let $V \in M_4$ be a unitary matrix with its first two columns $v_1$ and $v_2$ satisfying

$$\text{span}\,\{v_1, v_2\} = \text{span}\,\{x_1, x_2\}.$$

Then we know that both

$$(V^*XV)^t \quad \text{and} \quad (V^*YV)^t$$

have their last two columns being the zero column. Applying Lemma 2.2(b), the problem is reduced to the case $n = 2$ and, as $(X, Y)$ is maximal if and only if $(X^t, Y^t)$ is maximal, the claim follows easily.

Now suppose $y_3$ and $y_4$ are linearly dependent. Then we can find a unitary matrix $V \in M_4$ of the form $I_2 \oplus W$ such that the last column of $(V^*YV)^t$ is the zero column. Notice, that the last column of $(V^*XV)^t$ is still the zero column. Thus, by Lemma 2.2(b), the problem is trimmed to $n = 3$. □

We are left with the task of proving the theorem for $n = 3$. This is the last small step, but also the most elaborate.

**Proposition 3.7.** *Theorem 3.1 is true for* $3 \times 3$ *matrices* $X$ *and* $Y$.

**Proof.** By Corollary 3.4 (and mediately Propositions 2.1, 2.3 and 2.4) we assume that

$$\operatorname{rank}(\alpha X + \beta Y + \gamma Z) = 2 \quad \text{for all } \alpha, \beta, \gamma \in \mathbf{C} \text{ not all zero.} \tag{7}$$

As rank $X = 2$, upon unitary similarity on $X$, $Y$ and $Z$, we may assume

$$X = (x_1, x_2, 0), \quad Y = (y_1, y_2, y_3), \quad Z = (z_1, z_2, z_3),$$

with $x_i, y_i, z_i \in \mathbf{C}^3$. Then, Lemma 2.5 ensures

$$y_3, z_3 \in \operatorname{span}\{x_1, x_2\}. \tag{8}$$

If $y_3$ and $z_3$ are linearly dependent, then there exists a nonzero linear combination $\beta Y + \gamma Z \neq O$ such that its last column is the zero column. By Proposition 2.4, the pair $(X, \beta Y + \gamma Z)$ is also maximal. Lemma 2.2(b) yields

$$X = X_0 \oplus (0) \quad \text{with } X_0 \in M_2.$$

As $(X, Y)$ is maximal, Lemma 2.2(a) gives the desired

$$Y = Y_0 \oplus (0) \quad \text{for some } Y_0 \in M_2.$$

Now assume

$$y_3 \text{ and } z_3 \text{ are linearly independent.} \tag{9}$$

We will deduce a contradiction. In order to do this, we distinguish two cases.

**Case 1:** Assume that both $y_1, z_1 \in \operatorname{span}\{x_1, x_2\}$ or both $y_2, z_2 \in \operatorname{span}\{x_1, x_2\}$. Without loss of generality suppose $y_1, z_1 \in \operatorname{span}\{x_1, x_2\}$.

Assume further $y_2 \in \operatorname{span}\{x_1, x_2\}$ (or $z_2 \in \operatorname{span}\{x_1, x_2\}$). We consider the matrix $Y$ (or $Z$ in case $z_2 \in \operatorname{span}\{x_1, x_2\}$). Together with (8), we have $y_1, y_2, y_3 \in \operatorname{span}\{x_1, x_2\}$. Let $V \in M_3$ be a unitary matrix having its last column orthogonal to $x_1$ and $x_2$. Then,

$$(V^*XV)^t \quad \text{and} \quad (V^*YV)^t$$

have their last columns being the zero column. Note that this pair is also maximal. By Lemma 2.2(b), we know that $(V^*XV)^t$ and $(V^*YV)^t$ are matrices in $M_2 \oplus (0)$. Because of rank $X$ = rank $Y = 2$ we have $\ker(V^*XV) = \ker(V^*YV)$ and consequently

$$\ker X = \ker Y.$$

As $Xe_3 = 0$ for $e_3 = (0, 0, 1)^t$, we get $y_3 = Ye_3 = 0$. This contradicts (9).

Now regard $y_2, z_2 \notin \operatorname{span}\{x_1, x_2\}$. Let us first consider $Y$. Here we have $y_1, y_3 \in \operatorname{span}\{x_1, x_2\}$ but $y_2 \notin \operatorname{span}\{x_1, x_2\}$. From (7), as rank $(\alpha X + Y) = 2$ for all $\alpha \in \mathbf{C}$, we obtain $y_1, y_3 \in \operatorname{span}\{x_1\}$. Similarly, $z_1, z_3 \in \operatorname{span}\{x_1\}$. Then, $y_3$ and $z_3$ are linearly dependent, again contradicting (9).

**Case 2:** For $i = 1, 2$, at least one of the vectors $y_i, z_i$ is not in $\operatorname{span}\{x_1, x_2\}$. Then, we easily deduce the existence of $\beta, \gamma \in \mathbf{C}$, $|\beta|^2 + |\gamma|^2 = 1$, such that the first two columns of

$$W = \beta Y + \gamma Z$$

are not in span $\{x_1, x_2\}$. Put $W = (w_1, w_2, w_3)$ with $w_i \in \mathbf{C}^3$. Note that $\|W\|_{\mathrm{F}} = 1$ and $(X, W)$ is maximal by Proposition 2.4. From (8) and (9) we know that $w_3 \in$ span $\{x_1, x_2\}$ is nonzero. We must have linear dependency of $w_1$ and $w_2$. Otherwise, rank $W = 3$ would conflict with (7). Let $V \in M_3$ be a unitary matrix of the form $A \oplus (1)$, where $A \in M_2$ is chosen such that the first column of $V^*WV$ is zero. We now consider the maximal pair $(V^*XV, V^*WV)$. For notation simplicity, write

$$V^*XV = (x_1, x_2, 0) \quad \text{and} \quad V^*WV = (0, w_2, w_3),$$

where $x_1, x_2, w_2, w_3 \in \mathbf{C}^3$ are nonzero. Note that we still have $w_3 \in \text{span}\{x_1, x_2\}$ and $w_2 \notin \text{span}\{x_1, x_2\}$. Then, $x_1$ and $w_3$ are linearly dependent. Otherwise, rank $(V^*XV + V^*WV) = 3$ gives a contradiction again. Apart from an appropriate scaling, we may then assume

$$V^*XV = \begin{pmatrix} a & d & 0 \\ b & -a & 0 \\ c & f & 0 \end{pmatrix}, \quad V^*WV = \begin{pmatrix} 0 & g & a \\ 0 & -c & b \\ 0 & h & c \end{pmatrix}$$

and

$$V^*(XW - WX)V = \begin{pmatrix} -bg - ac & 2ag - dc - af & a^2 + db \\ 0 & bg - fb & 0 \\ -hb - c^2 & cg - 2fc + ha & ac + fb \end{pmatrix}$$

due to property (ii) of Proposition 2.1(b). By a direct inspection of the maximal pair, we get

$$\begin{aligned}
0 &= 2\|X\|_{\mathrm{F}}^2\|W\|_{\mathrm{F}}^2 - \|XW - WX\|_{\mathrm{F}}^2 \\
&= 8\,|a|^2|c|^2 + 4\mathrm{Re}\, ag\overline{cd} + 4\mathrm{Re}\, ah\overline{cf} && \text{(10a)} \\
&\quad + 2|b|^2\mathrm{Re}\, f\overline{g} + 4|a|^2\mathrm{Re}\, f\overline{g} + 4|c|^2\mathrm{Re}\, f\overline{g} && \text{(10b)} \\
&\quad + 6\,|a|^2|b|^2 + 6\,|b|^2|c|^2 + 2\,|f|^2|g|^2 + 2\,|b|^4 + 3\,|a|^4 + 3\,|c|^4 \\
&\quad + |b|^2|d|^2 + |b|^2|h|^2 - 2\mathrm{Re}\, a^2\overline{bd} - 2\mathrm{Re}\, c^2\overline{bh} && \text{(10c)} \\
&\quad + 3\,|a|^2|h|^2 + 3\,|c|^2|d|^2 + |a|^2|f|^2 + |c|^2|g|^2 \\
&\quad - 2\mathrm{Re}\, ac\overline{bf} - 2\mathrm{Re}\, ac\overline{bg} - 2\mathrm{Re}\, af\overline{cd} - 2\mathrm{Re}\, ah\overline{cg} && \text{(10d)} \\
&\quad + 2\,|a|^2|d|^2 + 2\,|c|^2|h|^2 + 2\,|d|^2|g|^2 + 2\,|d|^2|h|^2 + 2\,|f|^2|h|^2,
\end{aligned}$$

where Re $z$ denotes the real part of the complex number $z$.

We are going to examine several lines of the formula above. First observe

$$\text{(10a)} = 8\,|a|^2|c|^2 + 4\mathrm{Re}\, a\overline{c}(g\overline{d} + h\overline{f}) = 8\,|a|^2|c|^2 + 4\mathrm{Re}\, a\overline{c}(-\overline{a}c) = 4\,|a|^2|c|^2,$$

since $V^*XV$ and $V^*WV$ are orthogonal by Proposition 2.1(b)(iii). By usage of the elementary inequalities

$$\begin{aligned}
&\mathrm{Re}\,(xy) \geqslant -|xy| \quad (x, y \in \mathbf{C}), \\
&2xy \geqslant -(x^2 + y^2) \quad (x, y \in \mathbf{R}) \quad \text{and} \\
&(x + y)^2 \leqslant 2(x^2 + y^2) \quad (x, y \in \mathbf{R}),
\end{aligned}$$

we obtain

$$\begin{aligned}
\text{(10b)} &= 2 \cdot 2\left(|a|^2 + |c|^2 + \frac{|b|^2}{2}\right)(\mathrm{Re}\, f\overline{g}) \\
&\geqslant 2 \cdot \left(-2\left(|a|^2 + |c|^2 + \frac{|b|^2}{2}\right)|f\overline{g}|\right) \\
&\geqslant -2 \cdot \left(\left(|a|^2 + |c|^2 + \frac{|b|^2}{2}\right)^2 + |f\overline{g}|^2\right)
\end{aligned}$$

$$= -2 \cdot \left( |a|^4 + |c|^4 + \frac{|b|^4}{4} + 2|a|^2|c|^2 + |a|^2|b|^2 + |b|^2|c|^2 + |f|^2|g|^2 \right),$$

$$\begin{aligned}
(10c) &\geqslant |b|^2|d|^2 + |b|^2|h|^2 - 2|a|^2|bd| - 2|c|^2|bh| \\
&\geqslant |b|^2|d|^2 + |b|^2|h|^2 - \left(|a|^4 + |bd|^2\right) - \left(|c|^4 + |bh|^2\right) \\
&\geqslant -|a|^4 - |c|^4,
\end{aligned}$$

$$\begin{aligned}
(10d) &\geqslant -2|af|\,(|bc| + |cd|) - 2|cg|\,(|ab| + |ah|) \\
&\geqslant -\left(|af|^2 + (|bc| + |cd|)^2\right) - \left(|cg|^2 + (|ab| + |ah|)^2\right) \\
&\geqslant -|af|^2 - 2|bc|^2 - 2|cd|^2 - |cg|^2 - 2|ab|^2 - 2|ah|^2.
\end{aligned}$$

Finally, we conclude from (10)

$$\begin{aligned}
0 \geqslant\ & 2\,|a|^2|b|^2 + 2\,|b|^2|c|^2 + \frac{3}{2}\,|b|^4 + |a|^2|h|^2 + |c|^2|d|^2 \\
&+ 2\,|a|^2|d|^2 + 2\,|c|^2|h|^2 + 2\,|d|^2|g|^2 + 2\,|d|^2|h|^2 + 2\,|f|^2|h|^2 \geqslant 0
\end{aligned}$$

and hence necessarily

$$b = 0, \quad ah = cd = 0 \quad \text{and} \quad ad = ch = dg = dh = fh = 0.$$

For $a = d = 0$ we have $\operatorname{rank} X = \operatorname{rank} V^*XV \leqslant 1$. Assuming $a = 0$ and $d \neq 0$ we get $c = g = h = 0$ and consequently $V^*WV = O$. For $a \neq 0$ we must have $d = h = 0$ and moreover $a\bar{c} = 0$ because of $V^*XV \perp V^*WV$ (i.e. $x_2 \perp w_2$). Now, $c = 0$ yields $\operatorname{rank} V^*WV \leqslant 1$. In any case, we are in contradiction to (7). □

Collecting Propositions 3.3–3.7, the proof of Theorem 3.1 is eventually complete. Note that Proposition 3.3 (and in consequence Corollary 3.4) is the key to the main result. However, with very little work we get a slightly weaker version in Proposition 3.5.

**Remark.** The statements in this section and their proofs can immediately be restated for the real case if "unitary matrix" is replaced by "orthogonal matrix". Remember, that the results from the previous section are still true for real matrices, whence the references to them may be kept.

## 4. Further aspects

In the present section we want to emphasize some issues hidden in the previous sections, hint at connections and interpretations, comment on generalizations, as well as to put forth problems for future investigations.

**Aspect 1** (*Maximal pairs and their linear combinations*).
In the proofs of Propositions 3.6 and 3.7 we met the condition

$$\operatorname{rank}(\alpha X + \beta Y + \gamma Z) = 2 \quad \text{for all } \alpha, \beta, \gamma \in \mathbf{C} \text{ not all zero} \tag{11}$$

and often went into a dead-end subsequently. Nevertheless in the first parts of both proofs, we reduced the problem to $n = 2$ directly, rather than obtaining a contradiction. So, we are left with the question, whether (11) may hold for a maximal pair $(X, Y)$ of $2 \times 2$ matrices. We now prove that this is not possible!

By (11), any non-trivial linear combination of $X, Y$ and $Z$ is nonsingular. However, one easily shows that there are nonzero $\alpha, \beta \in \mathbf{C}$ with

$$\det(\alpha X + \beta Y) = 0.$$

More precisely, by help of Proposition 2.1(a), we only need to investigate rank two matrices

$$X = \begin{pmatrix} a & b \\ c & -a \end{pmatrix} \quad \text{and} \quad Y = \begin{pmatrix} e & f \\ g & -e \end{pmatrix}$$

with $X \perp Y$. Fixing $\beta = 1, \det(\alpha X + Y)$ is a polynomial of order two in $\alpha$. Observe, that $\operatorname{rank} X = 2$ causes the coefficient of $\alpha^2$ to be nonzero. So, we will find a zero $\alpha \in \mathbf{C}$ and get a contradiction.

It is well known [1] that the maximum number of $2 \times 2$ real matrices whose nontrivial real linear combinations are nonsingular is two. Thus, if one considers (11) for real matrices, we have the contradiction without the necessity for an investigation of the particular determinant.

This result substantiates the importance of Corollary 3.4 for the proof of Theorem 3.1, as in fact already all maximal pairs are covered at that point.

**Aspect 2** (*Necessary vs. sufficient conditions*).
Property (iv) of Proposition 2.1(b) requires that, for any maximal pair $(X, Y)$, the matrix $X$ is orthogonal to all powers of $Y$. However, for $2 \times 2$ matrices, which are tackled by Proposition 2.1(a), we have no such condition. Well, there is no special demand, as the criterion is automatically fulfilled. For this, observe for matrices of order two, that $Y^2$, $Y$ and $I_2$ are linearly dependent due to the Cayley–Hamilton theorem [5, p. 86]. The latter says that the characteristic polynomial

$$\chi_Y(t) = \det(tI_2 - Y) = at^2 + bt + c$$

is annulling for $Y$, i.e. $\chi_Y(Y) = O$. Hence,

$$0 = \operatorname{tr} X = \langle X, I_2 \rangle \quad \text{and} \quad 0 = \langle X, Y \rangle \quad \text{yield } 0 = \langle X, Y^2 \rangle.$$

In view of this aspect and the discussion after Example 2.7 it becomes clear that condition (i) of Theorem 3.2 implies both properties (i) and (iv) of Proposition 2.1(b). Moreover, it sharpens them in a suitable fashion resulting in a sufficient condition.

**Aspect 3** (*Geometric interpretations and algebraic connections*).
Part (vi) of Theorem 3.2 in [4] established an inequality for sums of vector products (in $\mathbf{R}^3$ or $\mathbf{C}^3$) with a proof based on (1). Additionally, Remark 3.4 of [4] bounded the squared norm of the commutator by twice the area of the rhomb spanned by $\|Y\|_F X$ and $\|X\|_F Y$. We want to point out another geometric/algebraic link.

Theorem 3.1 restricts the equality cases of (1) essentially to $2 \times 2$ matrices and Proposition 2.1(a) moreover tells us that such maximal pairs consist of two orthogonal elements in the Lie algebra $sl(2, \mathbf{C})$ of zero trace $2 \times 2$ matrices.

Set

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad X_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad X_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

It is not hard to see that $\{H, X_+ X_-\}$ is an orthonormal basis of $sl(2, \mathbf{C})$. One easily checks the equations

$$[H, X_+] = \sqrt{2} X_-, \quad [H, X_-] = -\sqrt{2} X_+, \quad [X_+, X_-] = \sqrt{2} H.$$

These circles of a maximal pair $(X_+, X_-)$ and (the adjoint of) their commutator appear in connection with Proposition 2.4.

Now, decompose two elements $A, B \in sl(2, \mathbf{C})$ by

$$A = \alpha_1 H + \alpha_2 X_+ + \alpha_3 X_- \quad \text{and} \quad B = \beta_1 H + \beta_2 X_+ + \beta_3 X_-,$$

with $\alpha_i, \beta_i \in \mathbf{C}$. Then, their commutator is given by the formal determinant

$$\begin{aligned} [A, B] &= \sqrt{2} \cdot \begin{vmatrix} H & X_+ & X_- \\ \alpha_1 & \alpha_2 & \alpha_3 \\ \beta_1 & \beta_2 & \beta_3 \end{vmatrix} \\ &= \sqrt{2} \cdot \left( \begin{vmatrix} \alpha_2 & \alpha_3 \\ \beta_2 & \beta_3 \end{vmatrix} H - \begin{vmatrix} \alpha_1 & \alpha_3 \\ \beta_1 & \beta_3 \end{vmatrix} X_+ + \begin{vmatrix} \alpha_1 & \alpha_2 \\ \beta_1 & \beta_2 \end{vmatrix} X_- \right). \end{aligned}$$

So, except for the constant $\sqrt{2}$, the Lie product $[A, B]$ behaves like the usual cross product in $\mathbf{C}^3$. There, in terms of the Euclidean norm, we further have

$$\|x \times y\|^2 = \|x\|^2\|y\|^2 - |\langle x, y\rangle|^2$$

with the usual inner product $\langle x, y\rangle$. In that way, we can relate the constant $\sqrt{2}$ and the orthogonality condition on $A$ and $B$ (see Proposition 2.1(b)(iii)) to the algebraic properties of the Lie product via

$$\|[A, B]\|_{\mathsf{F}}^2 = 2\left(\|A\|_{\mathsf{F}}^2\|B\|_{\mathsf{F}}^2 - |\langle A, B\rangle|^2\right).$$

Introducing the tensor product identity

$$\|A \otimes B - B \otimes A\|_{\mathsf{F}}^2 = 2\left(\|A\|_{\mathsf{F}}^2\|B\|_{\mathsf{F}}^2 - |\langle A, B\rangle|^2\right),$$

we see the inequality

$$\|AB - BA\|_{\mathsf{F}}^2 \leqslant \|A \otimes B - B \otimes A\|_{\mathsf{F}}^2,$$

that was shown in Theorem 3.1 of [4], to hold as an equality for all elements in $sl(2, \mathbf{C})$ and not only for maximal pairs.

**Aspect 4** (*Counting on restrictions*).
Investigations in [3] demonstrated that the equality cases of (1) can hardly be attained by probability experiments and that the chance for such an event is decreasing with increasing matrix order $n$. Necessary condition (i) in Proposition 2.1(b) enforces rank not greater than two for matrices that are part of a maximal pair, restricting us to a set of measure zero (for $n \geqslant 3$). This is an explanation for that behaviour and at first glance it's not a big jump from Proposition 2.1(b) to the characterization in Theorem 3.2. However, there is a huge gap in quality between the two results. The right choice for recognizing this is to look at both results in terms of degrees of freedom.

An $n \times n$ matrix has $n^2$ entries and hence, for any pair we need to fix $2n^2$ variables. First, investigate condition (i) of Proposition 2.1(b). We used several times that a rank two matrix (upon unitary similarity) can be written as $X = (x_1, x_2, 0, \ldots, 0)$ with columns $x_1, x_2 \in \mathbf{C}^n$, which leaves us only with $2n$ out of $n^2$ degrees of freedom. As the similarity is not simultaneously, the second matrix $Y$ does not necessarily follow the pattern of $X$. But, by writing

$$Y = \begin{pmatrix} y_1 & y_2 \end{pmatrix} \begin{pmatrix} y_3^t \\ y_4^t \end{pmatrix},$$

with $y_i \in \mathbf{C}^n$, we are restricted to $4n$ additional degrees of freedom. Note that by appropriate scaling conditions, we could moreover fix a constant number of variables. Now, properties (ii) and (iii) similarly discard three degrees. In addition, by an argumentation analogous to Aspect 2, property (iv) will determine not more than $2n$ variables. So, basically (up to an additive constant) we are left with $4n$ degrees of freedom by the necessary conditions.

In contrast to this, condition (i) of Theorem 3.2 permits only eight degrees of freedom, which are even reduced to five by conditions (ii) and (iii). Here, the number of variables is constant and not dependant of the order $n$.

**Aspect 5** (*Generalizations to other norms*).
In [9], analogues of (1) with the Schatten $p$ and vector $p$ norms (i.e. $p$ norms on the singular values or entries of the matrix) instead of the Frobenius norm were investigated:

$$\|[X, Y]\|_p \leqslant C_p\|X\|_p\|Y\|_p. \tag{12}$$

Note that $\|X\|_{\mathsf{F}} = \|X\|_2$ for both types of norms. Moreover, characterizations of the appropriate maximality were given for $p < 2$.

In the case of the Schatten norms, the constant $C_p$ in (12) is given by $2^{1/p}$. Further, in any Schatten $p$ maximal pair, both matrices must have rank one. Hence, by analogy to Example 2.7, Theorem 3.1 is valid here, too.

For the vector norms, the same constant in (12) is obtained. But, in contrast to the Schatten norms, there is basically only one maximal pair, namely $(X_+, X_-)$ from Aspect 3. As these norms are not unitarily invariant, it is not adequate to question the validity of Theorem 3.1 in this case.

If we regard $p > 2$, the two norm classes behave differently. The necessary constants in (12) are given by $2^{1-1/p}$ for the Schatten $p$ norms and $2^{1-1/p}n^{1-2/p}$ for the vector $p$ norms of even-dimensional $n \times n$ matrices. For odd dimensions, the constant is only bounded from above by that value, but very close to it. Characterizations of these maximal pairs and a possible adaption of Theorem 3.1 are still subject of research.

**Aspect 6** (*Building maximal pairs*).
In Lemma 2.2, we applied block structures in order to get statements about maximality. As the Schatten norms are unitarily invariant, there is a good chance that an approach similar to the one we have done for the Frobenius norm (i.e. $p = 2$) may also work for $p \neq 2$. However, so far the efforts produced only estimates that are not tight enough to prove an adaption of Lemma 2.2.

One may consider other special block matrices with that aim. First, think about

$$X = \begin{pmatrix} A & A \\ A & A \end{pmatrix} \quad \text{and} \quad Y = \begin{pmatrix} E & E \\ E & E \end{pmatrix}.$$

It is easy to check, that $(X, Y)$ is maximal if and only if $(A, E)$ is maximal. Since

$$\begin{pmatrix} I_n/\sqrt{2} & I_n/\sqrt{2} \\ I_n/\sqrt{2} & -I_n/\sqrt{2} \end{pmatrix} \begin{pmatrix} A & A \\ A & A \end{pmatrix} \begin{pmatrix} I_n/\sqrt{2} & I_n/\sqrt{2} \\ I_n/\sqrt{2} & -I_n/\sqrt{2} \end{pmatrix} = \begin{pmatrix} 2A & O \\ O & O \end{pmatrix},$$

this assertion may further be transferred to the $p$ maximality with respect to the Schatten norms. The claim cannot be true for the vector $p$ norm if $p < 2$, as the matrices $X$ and $Y$ would no longer admit only one nonzero entry. However, if $p > 2$ and $n$ is even, then the assertion holds. Indeed, we have for vector $p$ maximal pairs $(A, E)$

$$\frac{\|[X,Y]\|_p^p}{\|X\|_p^p\|Y\|_p^p} = \frac{4\|2[A,E]\|_p^p}{4\|A\|_p^p 4\|E\|_p^p} = \frac{2^p}{4} \cdot 2^{p-1}n^{p-2} = 2^{p-1}(2n)^{p-2},$$

which is the maximality of $(X, Y)$.

Similarly, one should investigate

$$X = \begin{pmatrix} A & O \\ O & A \end{pmatrix} \quad \text{and} \quad Y = \begin{pmatrix} E & O \\ O & E \end{pmatrix}.$$

It turns out that the maximality of $(A, E)$ does not imply the maximality of $(X, Y)$ in general. Such an assertion holds only for the two $\infty$ norms. Nevertheless, this structure is of particular interest, as it demonstrates the existence of maximal pairs containing matrices with rank greater than two. We conjecture that except for $p = \infty$, the Schatten and vector $p$ maximality requires low rank matrices. So, block diagonal structures of more than one non-trivial matrix should not be suitable for exploration.

**Aspect 7** (*Varying the norm indices*).
There are attempts for further generalization of the Schatten $p$ norm inequality (12) by waiving the restrictive condition for usage of the same norm three times and regard

$$\|[X,Y]\|_p \leqslant C_{p,q,r}\|X\|_q\|Y\|_r$$

for not necessarily equal Schatten $p, q$ and $r$ norms. In [2], the conjecture was raised that in the case $p = q$,

$$C_{p,p,r} = 2^{\max(1/p,1-1/p,1-1/r)}.$$

This is confirmed partially by the bounds for the special case $p = q = r$ mentioned in Aspect 5. Moreover, the constant has been proven for $p = 2$ (but $r$ arbitrary) in [2] by introducing the concept of variance, known from probability theory, for matrices and linking it to elements of planar geometry, especially the notion of radius.

Actually, Audenaert obtained the value of $C_{2,2,r}$ by proving the slightly stronger inequality

$$\|[X,Y]\|_2 \leqslant \sqrt{2}\|X\|_2\|Y\|_{(2),2}. \tag{13}$$

Here, the Schatten 2 norm $\|X\|_2 = \|X\|_{\mathsf{F}} = \sqrt{\sigma_1^2 + \cdots + \sigma_n^2}$ can be calculated as the Euclidean norm of the vector $(\sigma_1, \ldots, \sigma_n)$ of decreasingly ordered singular values of $X$ and $\|X\|_{(2),2} = \sqrt{\sigma_1^2 + \sigma_2^2}$ is a Schatten/Ky Fan mixture norm, respecting only the two largest singular values. The validity of (13) is consistent with our observations regarding the equality states of (1), telling that matrices in maximal pairs have at most two nonzero singular values and hence $\|Y\|_{(2),2} = \|Y\|_2$.

Symmetry considerations and numerical tests give hope that even

$$\|[X,Y]\|_2 \leqslant \sqrt{2}\|X\|_{(2),2}\|Y\|_{(2),2}$$

is true. However, the example

$$X = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \oplus \cdots \oplus \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad Y = X^t$$

demonstrates that $\sqrt{2}$ cannot be guaranteed and further that there is no constant independent of dimension. Note that the example above acts as a counter example only for matrix orders $n \geqslant 6$. Nevertheless, a similar inequality that was raised in [4],

$$\|[X,Y]\|_{(2),2} \leqslant \sqrt{2}\|X\|_{(2),2}\|Y\|_{(2),2}$$

is still under investigation. Whereas (13) is respecting the whole range of singular values on both sides of the inequality, the last inequality simply withdraws growths like the one seen in the example.

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